Chloranil

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 3.97e-13 cm3/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.20e-01

Confidence level: 7.12e-01

Nearest Neighbors from the Training Set

Image not found
Dimethyl sulfate
Measured: 5.00e-13
Predicted: 4.96e-13

Image not found
Diethyl sulfate
Measured: 1.80e-12
Predicted: 1.55e-12

Image not found
Propylene dinitrate
Measured: 3.20e-13
Predicted: 3.59e-13

Image not found
2,3-Butanedione
Measured: 2.38e-13
Predicted: 3.43e-13

Image not found
Peroxyacetyl nitrate
Measured: 1.00e-13
Predicted: 9.98e-14